Benzeneacetic acid, 4-hydroxy-156-38-7 | DTXSID5059745

100-30-7	D1791039743	

Model Performance

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Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 4.23

Global applicability domain: Inside

Local applicability domain index: 4.28e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

Image not found

2,2-Dimethylpropanoic acid

Measured: 2.29 Predicted: 2.74

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Phenylphosphinic acid

Measured: 6.03 Predicted: 4.42

Image not found

Benzoic acid, 4-(methylamino)-

Measured: 2.40 Predicted: 4.00

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3-Nitrobenzoic acid Measured: 7.08 Predicted: 3.63

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Dalapon-sodium Measured: 7.24 Predicted: 5.61